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Solution of finite moment problem using density matrix type of expansion

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Abstract : The density matrix type of expansion is used to find the single particle density which reproduces the given low order moments. The connection of the present formulation with an earlier well-known method is shown. Explicit expressions for the density are worked out for the first few given low order moments. Possible future applications in different branches of physics are mentioned.

Keywords : Probability density formulations, few moments problem.

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1. Introduction

The problem of constructing the probability density function from the known few low order moments is fairly well known. Several methods have been suggested in the past for the solution of this problem, *e.g.*, the method based on the principle of maximum entropy [1] and the method of successive approximations developed by Kryachko and Koga [2] using the pair of Hankel transforms.

Recently, it has been shown that many problems of physical interest like classical hard sphere equation of state [3] and solution of certain integral equations can also be solved using the probability density constructed from the first few low order moments. This has created new interest in the problem of finding the probability density from its first few low order moments. In the present work we would like to show how an expansion which is used in the problem of density matrix [4] can be utilized to find an expression for the single particle density if its first few order moments are known. It will be shown later that the final expression obtained in the present formulation is quite simple and its zeroth approximation itself gives a distribution which is quite often used in a many-nucleon system. We describe the essential formulation in Section 2. In Section 3 we shew the connection with the earlier work. We work out specific distributions for low order moments in Section 4. Conclusions and possible future applications are discussed in Section 5.

2. Formulation

In the present formulation we shall consider a spherically symmetric density $\rho(r)$ and assume that a finite set of its even moments are known. The spherically symmetric form factor $f(k)$ and the density $\rho(r)$ are related to each other by a pair of Hankel transform as [2]

$$f(k) = 4\pi \int_0^\infty dr\, r^2\, \rho(r) j_0(kr), \tag{1a}$$

$$\rho(r) = \frac{1}{2\pi^2} \int_0^\infty dk\, k^2 f(k) j_0(kr), \tag{1b}$$

where j_0 is the spherical Bessel function of order zero [5]. The even moments of $\rho(r)$ are given by

$$< r^{2n} > = 4\pi \int_0^\infty dr\, r^{2n+2}\, \rho(r) \tag{2}$$

Thus $\rho(r)$ is normalized such that

$$4\pi \int_0^\infty dr\, r^2\, \rho(r) = < r^0 > = N, \tag{3}$$

N being the total number of particles in the system.

As emphasized by Kryachko and Koga [2], if one expands $j_0(kr)$ in (1a) using the usual series expansion [5] and writes $f(k)$ in terms of the few low order moments of $\rho(r)$, then the substitution of this $f(k)$ in (1b) gives rise to a divergent integral. To derive an expression for $\rho(r)$ which avoids this problem, we use the following identity which is used in the density matrix formulation [4]

$$j_0(kr) = \sum_{n=0}^{\infty} (-1)^n (4n+3) \frac{j_{2n+1}(ak)}{(ak)} \frac{P_{2n+1}(r/a)}{(r/a)} \tag{4}$$

where a is a parameter. As will be shown later when specific examples are given, the parameter a plays the role of a cut-off radius for the density. With the introduction of the parameter a, all the relevant integrals remain finite.

It should be recalled here that Wigner's density matrix formulation [4] is also called the alternative formulation of Quantum Mechanics. It has features which can profitably be used in the study of many-body physics. In the present context, since a truncated form of eq. (4) containing spherical Bessel functions will be employed, this will physically mean that one is dealing with short range interactions and thus will be most suitable for a many-nucleon system. This is borne out later when we give the zeroth order approximation.

Now suppose that a number of low-order moments of $\rho(r)$ were known, then we have to use the truncated form of the identity (4) in $f(k)$. By expanding the spherical Bessel function $J_{2n+1}(ak)$ and Legendre polynomial $P_{2n+1}\frac{r}{a}$ one could easily check that $f(k)$ gives exactly the chosen low-order moments. Now as in Kryachko and Koga [2], this approximate form of $f(k)$ given by

$$f(k) = \sum_{n=0}^{M} A_n \frac{j_{2n+1}(ak)}{(ak)}, \tag{5}$$

when substituted in (1b), makes it possible to carry out integration over k and gives the following form for the density $\rho(r)$

$$\rho(r) = \frac{1}{4\pi a^3} \sum_{n=0}^{M} (-1)^n A_n \frac{P_{2n+1}(r/a)}{(r/a)}, \; r \le a, \tag{6a}$$

$$\rho(r) = 0 \qquad\qquad r > a, \tag{6b}$$

where the constants A_n, a are functions of the set of the lowest $M + 2$ moments. Expressions (6a), (6b) are the desired expressions for the approximate single particle density which correctly reproduces the few given low order moments.

3. Connection with the earlier work

In the literature, it has not been shown that one could also derive some of the earlier approximate distributions using the exact relations (1). Here, we show the connection with one of the earlier methods which has been quite often used in the problem of moments.

We start from the integral representation of the spherical Bessel function [5] j_0 which is given by

$$j_0(kr) = \frac{1}{2}\int_{-1}^{1} dt \, \exp(it\, kr), \tag{7}$$

using the generating function for the Hermite polynomials

$$\exp(-\xi^2 + 2x\xi) = \sum_{n=0}^{\infty} \frac{H_n(x)}{(n!)} \xi^n, \tag{8}$$

we can write $j_0(kr)$ as

$$j_0(kr) = \frac{1}{2}\int_{-1}^{1} dt \, \exp(-k^2) \sum_{\mu=0}^{\infty} \frac{H_{2\mu}\left(\frac{1}{2} tr\right)}{(2\mu)!} (-1)^{\mu} (k^2)^{\mu}. \tag{9}$$

Now suppose only the first $M + 1$ moments of $\rho(r)$ were known, then putting (9) into (1a) we can write

$$f(k) = \exp(-k^2) \sum_{\mu=0}^{M} A_{\mu} (k^2)^{\mu}, \tag{10}$$

where A_μ is given in terms of the first few lowest moments of $\rho(r)$ as

$$A_\mu = \sum_{s=0}^{\mu} \frac{\Gamma(-\mu+S)}{\Gamma(-\mu)} \frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3}{2}+S\right) S!} \frac{\langle r^{2S} \rangle}{2^{2S}} \tag{11}$$

Substituting expression (10) in expression (1b), we find that the density $\rho(r)$ in terms of the first few order moments is given by

$$\rho(r) = (2\pi)^{-2} \exp\left(-\frac{1}{4} r^2\right) \sum_{\mu=0}^{M} A_\mu \Gamma\left(\mu + \frac{3}{2}\right) M\left(-\mu, \frac{3}{2}, \frac{r^2}{4}\right), \tag{12}$$

where M is the confluent hypergeometric function [5].

Since the confluent hypergeometric function has its first parameter a negative integer, it is a polynomial in r^2. Thus expresion (12) reproduces the well-known approximation of fitting a density with a Gaussian multiplied by a polynomial [6].

4. Explicit form of the density

We shall now give explicit form of $\rho(r)$ in terms of the moments using the formulation described in section 2. We start with the zeroth order problem in which the two moments $<r^0>$, $<r^2>$ are known. This means $\rho(r)$ is of the form.

$$\rho(r) = \frac{A_0}{4\pi a_0^3} \quad r \le a, \tag{13a}$$

$$\rho(r) = 0 \qquad r > a, \tag{13b}$$

The two constants A_0, a can easily be written down in terms of $<r^0>$, $<r^2>$, the final expression being

$$\rho(r) = \frac{3}{4\pi} \cdot <r^0> \left[\frac{5}{3}\frac{<r^2>}{<r^0>}\right]^{-\frac{3}{2}}$$

$$r \le \left[\frac{5}{3}\frac{<r^2>}{<r^0>}\right]^{\frac{1}{2}}, \tag{14a}$$

$$\rho(r) = 0, \quad r > \left[\frac{5}{3}\frac{<r^2>}{<r^0>}\right]^{\frac{1}{2}} \tag{14b}$$

As was remarked in the introduction this is the earliest form of the density of nucleons [7]. Thus the zeroth approximation of the present formulation gives a single particle density which is quite often used in many-nucleon system. This form is also used in the Fermi gas model [8].

We next give the density $\rho(r)$ when the three moments $<r^0>$, $<r^2>$ and $<r^4>$ are known. It is convenient to introduce new constants and write $\rho(r)$ given by (6a) and (6b) as

$$\rho(r) = \frac{1}{4\pi a^3}\left[b_0 - b_1\left(\frac{r}{a}\right)^2\right], \quad r \le a, \tag{15a}$$

$$= 0, \text{ otherwise.} \tag{15b}$$

It is easy to see that a, b_0, b_1 are given by the following expressions

$$a^2 = \frac{7}{3}\frac{<r^2>}{<r^0>}\left[1 - \sqrt{1 - \frac{27}{35}\gamma}\right], \tag{16a}$$

$$b_0 = \frac{75}{4}<r^0>\left(1 - \frac{7}{5}\,\frac{<r^2>/<r^0>}{a^2}\right), \tag{16b}$$

$$b_1 = \frac{105}{4}<r^0>\left(1 - \frac{5}{3}\,\frac{<r^2>/<r^0>}{a^2}\right), \tag{16c}$$

where

$$\gamma = \left(\frac{<r^4>}{<r^0>}\right)\left(\frac{<r^2>}{<r^0>}\right)^{-2} \tag{17}$$

Unlike the zeroth order density given by (14a), (14b), the density given by (15a), (15b) is not automatically positive. The condition $\rho(r) \ge 0$ for $r \le a$ is satisfied if the minus sign is used in the solution of the quadratic satisfied by a^2. This gives expression (16a) for the determination of a^2. Further, the ratio γ has the range $\frac{49}{45} \le \gamma \le \frac{35}{27}$. Because of the form of the approximate density distribution, it is always possible to find the range of the ration γ for which the distribution remains positive. In this way, the present formulation is better than many other approximate forms *e.g.* the one mentioned in Section 3 where one neither knows whether the distribution will remain positive for all γ ' s and if not so then how to find the range of γ for which the distribution remains positive.

Similarly one could work out explicit expressions for $\rho(r)$ if the set of moments is enlarged to four or more.

5. Conclusions

We have shown how the density matrix type of expansion can be used to obtain an expression for the single particle density which has a given set of low order moments. In the zeroth approximation it gives a step function as the density. It should be mentioned here that the zeroth approximation given by Kryachko and Koga gives a δ-function while the one obtained using the principle of maximum entropy gives a Gaussian function. At present there is no way to say which of the approximate forms of $\rho(r)$ is the best. In all cases one can calculate the higher moments and if one of these is known it could be used to see which of the approximate forms is better. The present formulation has the nice feature that one can explicitly see the positivity condition on $\rho(r)$ which some of the other approximations do not have, except the one obtained using the principle of maximum entropy which is always positive. However, it should be remembered that the integrals using this form are extremely difficult to work our analytically.

We have shown how Hankel transform formulation could be used to derive one of the well-known earlier approximation for probability density.

As shown in Section 4, even the zeroth approximation of the present formulation gives a distribution which is very often used in a many-nucleon problem. It will be interesting to see how it compares with other approximations when applied, *e.g.*, to the problem of hard sphere and hard-disc equations of state where one could easily work out all the necessary integrals analytically rather than numerically.

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